Investigating Effects of Spray Characteristics on Fuel-Air Mixture Formation

UNDERGRADUATE HONORS THESIS

Presented in Partial Fulfillment of the Requirements for Graduation with Honors Research Distinction in the Department of Mechanical and Aerospace Engineering at The Ohio State University

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Undergraduate Program in Mechanical Engineering

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2018

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Abstract

Fuel-air mixture formation is an important research topic in the internal combustion (IC) engine field with respect to fuel consumption and emissions of a vehicle. Spray characteristics have significant effects on fuel-air mixture formation. In this research, spray and fuel-air mixture formation processes in the gasoline direction injection (GDI) engine are simulated in the pre-built models in the commercial software Converge CFD with emphasis on the effects of spry characteristics on such processes. The focus is placed on the effects of the injector configuration and operating conditions. A pre-built model is modified by adding spray modeling including injector and nozzles. The shape of the nozzles is initially designed as an equilateral hexagon. To improve undesired spray characteristics observed in the simulation results, the shape of the nozzles is changed as an equilateral triangle and the overall angle of the nozzles is changed downward. To mimic the effects of the injection pressure and the geometry and investigate the effects of modeled evaporation rates, the droplet size and the transfer coefficients in the droplet evaporation model are adjusted. Results of this study ideally illustrate the working process, discrete phase modeling and relationship among different variables that substantially influence the stability, efficiency and emission. By changing the shape of nozzles, less fuel is sprayed on Intake Port. Adjusting droplet size and scaling parameters would optimize fuel-air mixture formation as less fuel sprayed on the equipment and the equivalence ratio distribution improves by the adjustment. However, while idealizing certain aspects of the fuel-air mixture formation, other issues emerge due to the change of parameters, which still need more work to optimize the case.

Dedication

Dedicated to the students at The Ohio State University

Acknowledgement

I am grateful to my advisor Dr. Seung Hyun Kim, who has provided me with this precious undergraduate research opportunity. Dr. Seung Hyun Kim has advised me throughout entire research process even during the break. Without his advising and encouragement, I could not have completed the first research project in my life.

I would also like to acknowledge Mr. Wei Wang, a PhD student working in the lab, who helps me understand concepts in the research and learn how to manipulate Converge CFD. I would also like to acknowledge Mr. Yunde Su, a PhD student working in the lab, who helps me with the operation system. Finally, I would like to thank Dr. Jung Hyun Kim for helping me, taking time reviewing my thesis, and serving as undergraduate thesis committee member.

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L	Liquid sheet length
θ	2θ spray cone angle
h	Liquid sheet thickness
X	Ratio of the cross-sectional area
A	Nozzle constant
$\dot{q}$	Liquid volume flowrate
P_{in}	Injection pressure
P_a	Ambient pressure
U	Relative velocity
V_0	Initial velocity
C_v	Dimensionless velocity coefficient
r_c	Radius of the new child droplet
a	Parent droplet radius
Λ	Wave-length of a surface
Ω	Maximum growth rate
C_f	Dimensionless constant
C_b	Dimensionless constant
C_k	Dimensionless constant
C_d	Dimensionless constant
ρ_g	Gas density
σ	Surface tension
r	Droplet radius
x	Displacement of the equator of the droplet from its equilibrium position
t_{bu}	Break-up time
C_{ZZ}	Dimensionless constant

r_{32} Sauter mean radius

K Ratio of energy of distortion and oscillation to the total energy in the fundamental mode

m_d Droplet mass

V_p Droplet velocity

C_D Drag coefficient

A_f Projection area of the droplet

ρ_1 Liquid density

μ_1 Liquid viscosity

$\emptyset_1$ Velocity potential

φ_1 Stream function

C_1 Integration constants

C_2 Integration constants

I_0 Modified Bessel functions

I_1 Modified Bessel functions

τ_{KH} KH model break-up time

B_1 Breakup time constant

D Mass diffusivity of liquid vapor in air

D_0 Related constants

n_0 Related constants

Abbreviations

IC Internal Combustion

CFD Computational Fluid Dynamics

DI Direct Injection

TAB Taylor analogy break-up

KH Kelvin-Helmholtz

1. Introduction

1.1 Motivation

Although the new technologies continue to be promoted, the demand for energy conservation is still driving vehicle manufactures to consider internal combustion (IC) engines since traditional vehicles powered by gasoline still take up a large portion of transportation. The demand for energy conservation related technique turns to be higher with the increasing need to reduce fuel consumption and gas emission produced by IC engines while more IC engine vehicles are under operation. In 2016, about 143.37 billion gallons of finished motor gasoline were consumed in the United States, a daily average of about 391 million gallons. [1] Currently, gasoline and diesel are still the main selections for power supply for objectives from vehicles to factories due to a relatively lower price, proven techniques and existing facilities. Fuel consumption and exhaust gas emissions have been a universal concern for long due to environmental protection and sustainable development.

Just like an optimized fuel injector while being signaled by the engine control unit, opening and spraying the pressurized fuel into an engine cylinder, advanced hardware can optimize the working process for IC engines. However, the techniques for hardware manufactures are always limited. In addition, pivotal factors applied to IC engines, which could be controlled manually, can also have a huge impact on the IC engine performance. These known factors which have not been calibrated perfectly and unknown factors which still need discovering can affect the entire performance and the consumption and emission outcome.

Fuel-air mixture formation is an important factor that has drastic influence on fuel consumption and gas emission. However, the formation of the fuel-air mixture is influenced by numerous factors including spray characteristics, which is controlled by ambient pressure, injector condition, flow condition including liquid break-up condition, evaporation condition and equivalence ratio. Although changes of some of these parameters do not have a conspicuous effect on spray characteristics, they have already given out a trend of idealized fuel-air mixture formation.

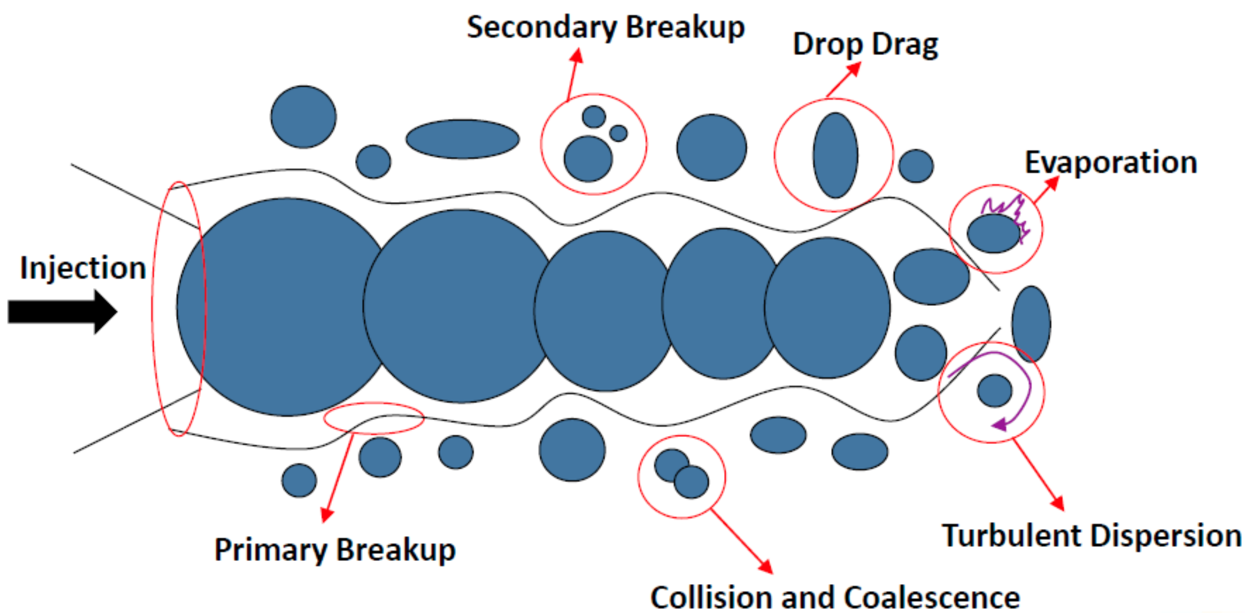

Figure 1 Schema of a spray analyzed by sub-grid modeling

There are numerous related researches that have been done on spray characteristics in terms of ambient pressure, droplet vaporization and other factors. In the previous studies, hollow-cone spray is analyzed by Reitz's wave break-up model, the

Taylor analogy break-up (TAB) model and the drag force model, as well as vapor phase transport equations, liquid balance equations, distribution functions and vapor-liquid equilibrium etc. In the research process, once a parameter is changed, even though certain aspect is improved, other aspects might turn to be worse. Regular numerical calculation cannot reach the comprehensive simulation. Therefore, models simulated by Converge CFD must be developed to investigate potential influence factor. In detail, using Converge CFD, the effects of spray characteristic on fuel-air mixture formation in a GDI engine is investigated. The angles of injector and nozzles, as well as the injection pressure are the primary parameters to investigate. The injection pressure influences the initial droplet sizes that are changed in the simulations.

1.2 Background

Instead of studying numerical calculation of the model, mixture formation processes inside a gasoline direct injection (GDI) engine is simulated to analyze the spray angle changed with ambient pressure. Converge CFD, a commercial software to simulate engine in-cylinder flows, applies the basic principle as the finite volume method (FVM) which breaks the whole model into a big amount of very tiny pieces and analyze the reaction of each element to the parameter changed in the system. With the model set up in the software, the liquid, injection, drop drag, liquid/ gas coupling and spray breakup will be simulated to calculate the droplet deformation, drag force, spray angle and equivalence ratio.

In computational simulation, the Kelvin-Helmholtz (KH) breakup model and the Rayleigh-Taylor (RH) breakup model are applied to simulate the droplet break-up scenario. In this research, the equations that come with the models are not applied since the software requires user to input several parameters only, which reduces a lot of work.

The Kelvin-Helmholtz breakup model considers the stability of a cylindrical, viscous, liquid jet of radius r_0 issuing from a circular orifice at a velocity U into a stagnant, incompressible, inviscid gas of density ρ_g. The liquid has a density ρ_1 and viscosity μ_1. A cylindrical polar coordinate system is used which moves with the jet. An arbitrary infinitesimal axisymmetric surface displacement of the form is imposed on the initially steady motion and it is thus desired to find the dispersion relation, which relates the real part of the growth rate to its wavenumber. In order to determine the dispersion relation, the linearized hydrodynamic equations for the liquid are solved with wave solution of the form

$$\emptyset_1 = C_1 I_0(k_{KH} r) e^{ik_{KH}Z + \omega_{KH} t}$$

$$\varphi_1 = C_2 r I_1(Lr) e^{ik_{KH}Z + \omega_{KH} t}$$

where $\emptyset_1$ and φ_1 are the velocity potential and stream function respectively. C_1 and C_2 are integration constants. I_0 and I_1 are modified Bessel functions of the first kind. $L^2 = k_{KH}^2 + \omega_{KH}/v_l$, and v_l is the liquid kinematic viscosity. The liquid pressure is obtained from the inviscid part of the liquid equations. The inviscid gas equations can be solved to obtain the fluctuating gas pressure at $\mathrm{r} = r_p$

$$p_g = -\rho_g \left(U - i\frac{\omega_{KH}}{k_{KH}} \right)^2 k_{KH} \eta \, \frac{K_0\left(k_{KH} r_p\right)}{K_1\left(k_{KH} r_p\right)}$$

where K_0 and K_1 are modified Bessel functions of the second kind and U is the relative velocity between the liquid and the gas. The linearized boundary conditions are mathematical statements of the liquid kinematic free surface condition, continuity of shear stress, and continuity of normal stress. With boundary condition, the desired dispersion relation could be obtained, which could also predict that a maximum growth rate exists for a given set of flow conditions.

In the KH model, the initial parcel diameters are set equal to the nozzle hole diameter d_0 and the atomization process of he relatively large injected blobs is modeled using the stability analysis for liquid jets. The breakup of the parcels and resulting drops is calculated by assuming that the breakup drop radius $r_c$is proportional to the wavelength of the fastest growing unstable surface wave. The rate of change of drop radius in a parent parcel is given by

$$\frac{dr_p}{dt} = -\frac{r_p - r_c}{\tau_{KH}}$$

where the breakup time τ_{KH} is given by

$$\tau_{KH} = \frac{3.726\ B_1 r_p}{\Lambda_{KH}\ \boldsymbol{\Omega_{KH}}}$$

The breakup time constant B_1 is related to the initial disturbance level on the liquid jet and has been found to vary from on injector to another.

The Rayleigh-Taylor breakup model is another model that considered to be responsible for droplet breakup other than the KH breakup mechanism. The unstable RT waves are thought to occur due to the rapid deceleration of the drops from the magnitude of the drag force. Typical implementations of the RT breakup model ignore both gas and liquid viscosity. In Converge CFD, the wavenumber corresponding to the maximum growth rate is solved for numerically using a bisection method.

2. Problem Formulation

The goal of this research is to evaluate and better understand how fuel-air mixture formation process is influenced by spray characteristics which are controlled by numerous factors adjusted manually. Accordingly, a systematic study of a representative fuel-air mixture formation in an IC engine is proposed. The study will be limited to parameters adjustment which might influence the fuel-air mixture formation and discovery of new factors that potentially influence the process. The steps to achieve the research goal are to:

(i) evaluate the numerical calculation and simulation done in previous literature and manual and get certain approximate values which are used in the computational simulation;

(ii) modify a pre-built model in Converge CFD by adding spray modeling which could specify the characteristics of injector;

(iii) design and adjust the shape of nozzles and scaling parameters to approach ideal fuel-air mixture which is evaluated by equivalence ratio;

To make this a tractable problem, this study will be restricted to the study of spray modeling parameter adjustment. The specific system generally is composed by an Intake Port, an Exhaust Port and a cylinder, as well as the injector added. Due to the complicacy of the system, the study will be restricted to specified IC engine with customized spray modeling. The spray modeling will be designed to approach the objectives as full combustion and ideal equivalence ratio. Ideal condition of the equipment is assumed.

The source of uncertainty considered in this research will be the situation as change of one parameter that could improve the performance in certain aspect might negatively influence other aspects in the model. The outcome of this study will be to identify the impact of the modification of these parameters on fuel-air mixture formation process under ideal condition. This work does not consider other practical situation the system might face, such as durability and environment condition.

3. Methodology

3.1 Spray Modeling Case Setup

Converge CFD is a commercial software which could model both gaseous and liquid sprays, involving state-of-art models for spray processes involving liquid atomization, drop breakup, collision and coalescence, turbulent dispersion, and drop evaporation. In terms of liquid sprays, Lagrangian solver is applied in Converge CFD to model discrete parcels and Eulerian solver is applied to model the continuous fluid domain. Parcels are also introduced into the domain at the injector, which presents a group of identical drops with same radius, velocity and temperature. Parcel is also the basic unit Converge solves instead of drop. Parcels experience the following process, primary breakup, secondary breakup, drop drag, collision and coalescence, turbulent dispersion and evaporation.

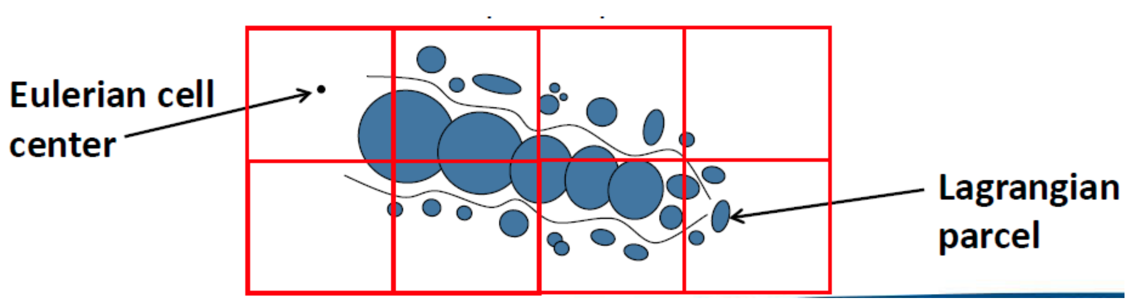

Figure 2 Schema of liquid sprays

In Converge CFD, spray modeling where spray related parameters could be changed is added by adjusting the setup option under physical models. Parcel is also setup by changing material species options. Simulation in the software assumes the parcel to be evenly distributed throughout the cone.

In the setup options, default values are applied for mass diffusivity constants.

$$\rho_{gas} D = 1.293 D_0 (\frac{T_{gas}}{273})^{n_0 - 1}$$

where D is the mass diffusivity of liquid vapor in air. Related constants D_0 and n_0 could be selected from the drop-down menu for common fuels.

In spray modeling, NTC numerical algorithm is applied for drop collision options and post collision outcomes is applied for collision/coalescence outcome options as default. Parcels can collide with parcels in the same cell only in typical simulation. However, Converge CFD reduces grid sensitivity since it has an adaptive collision mesh option, which means it allows parcel to collide with parcels in different cells. Dynamic drag model is used in this simulation since the drag coefficient calculation accounts for variation in the drop shape and invokes the TAB model to determine the distortion.

In this study, IC8H18 is selected as injected species and the mass fraction is adjusted as 1.0 since it is the only fuel injected.

An injector contains a group of nozzles that shares some of the same characteristics. An initial setup for the nozzle shape is equilateral hexagon which allows the fuel to spray in as many directions as possible and avoid the nozzle overlapping if there are too many nozzles coming out of the injector.

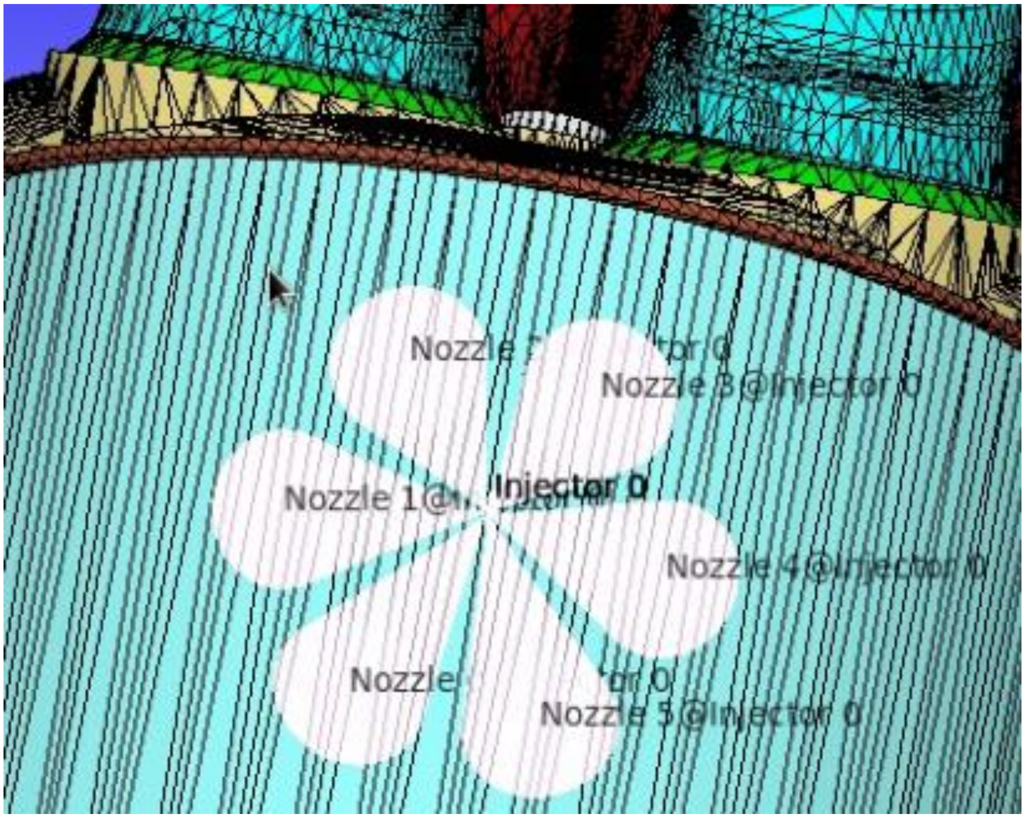

Figure 3 An injector with 6 nozzles in equilateral hexagon shape

Then, the position of the injector is move towards the center of the cylinder, a little bit offset of the center, and the nozzle shape is adjusted to be equilateral triangle.

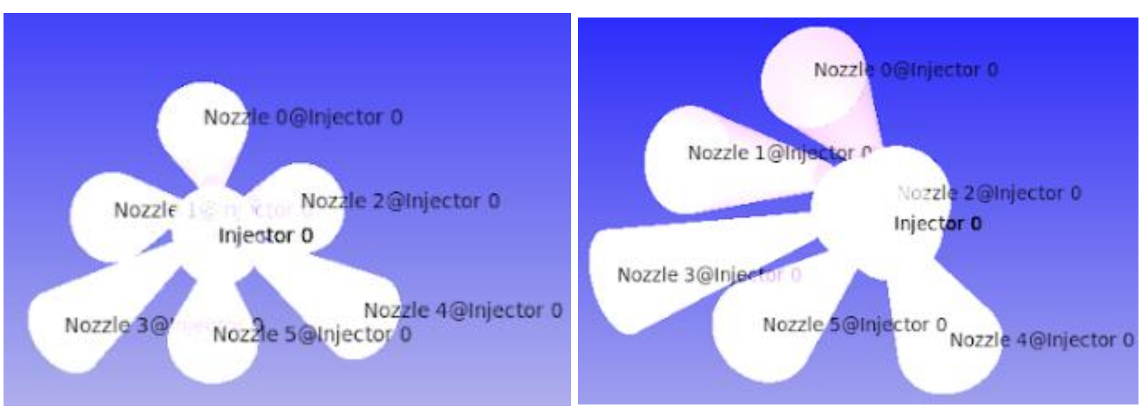

Figure 4 An injector with 6 nozzles in equilateral triangle shape

For a new case, the position of the injector is put back to the original place, the center of the injector entrance.

After applying all the possible and reasonable position of the injector and nozzle shape, the droplet size is further changed to discover the impact of the droplet size on fuel-air mixture formation. In the computational simulation, Kelvin-Helmholtz Breakup Model and Rayleigh-Taylor Breakup Model are applied to calculate the droplet breakup process. In KH model, with the default value for fraction of injected mass/parcel, shed mass constant, model velocity constant and model breakup time constant, the model size constant changes to be half of the reference value. In RT model, with default value for model breakup time constant and model breakup length constant, model size constant also changes to be half of the reference value.

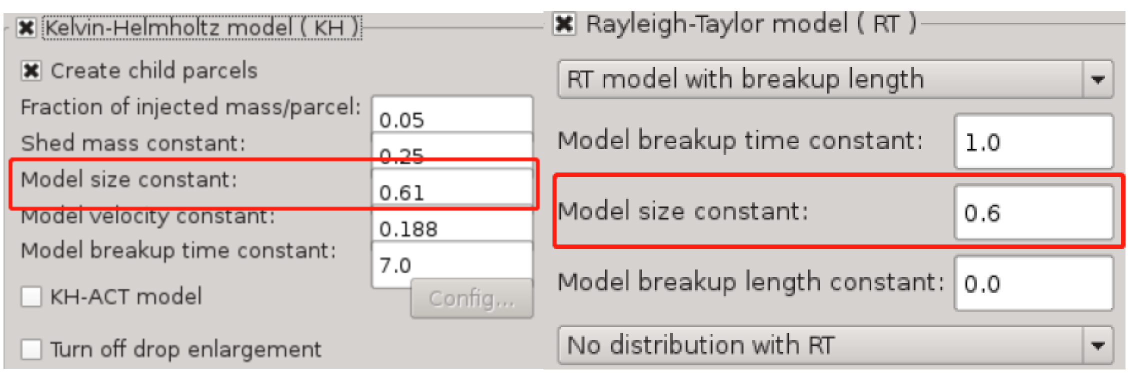

Figure 5 Setup for KH and RT model

Scaling factors including droplet heat transfer coefficient, droplet mass transfer coefficient, film heat transfer coefficient and film mass transfer coefficient are changed as 5 times as its reference value (from 1.0 to 5.0) due to the fact that after changing the nozzle shape (including angle and arrangement) and droplet size, the film on the liner, which means the fuel sprayed on it, is still at a relatively high value.

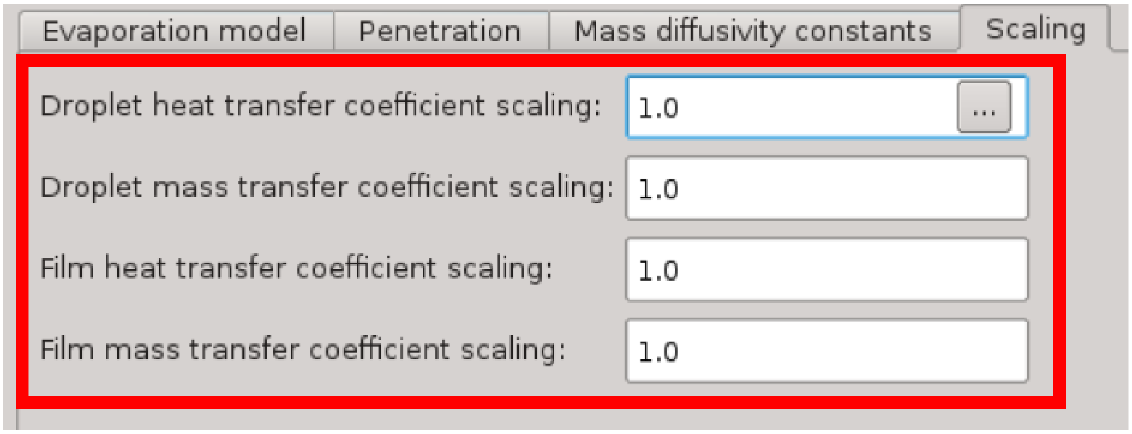

Figure 6 Setup for scaling parameters

After setting up all these parameters, the setup result is exported into *spray.in* file.

3.2 Spray Post-Processing

Converge CFD includes Pre-Processing, which is also referred as Case Setup as mention in 3.1, and Post-Processing, which refers to the process of utilizing the result data from output file produced during calculation process to generate plots and 3D vision model.

In Post-Processing interface, line plotting is applied to visualize the trend of variable changing. All the files including pressure, temperature and film could be shown with the crank angle as x-axis. The results of different cases could also be shown in the same plot to compare the results and amelioration of each case.

4. Analysis

4.1 Result by changing the nozzle shape and injector position

As shown in the previous section, the initial setup for nozzle shape is equilateral hexagon with all other parameters setup. After running the first case, although the case run successfully without errors, a large percentage of fuel is sprayed on the Intake Port (bound_id_8 in Converge CFD), which means the position of the injector, nozzle combination and overall angle are not appropriate for the case study. The legend in figure 7 indicates the line from case 1 to case 4. After changing the nozzle shape and injector position, as shown in figure 7, except for the first case, all the other results reduce from 3e-08 to 0, which means changing the nozzle shape and injector position works for reducing the fuel spraying on the Intake Port.

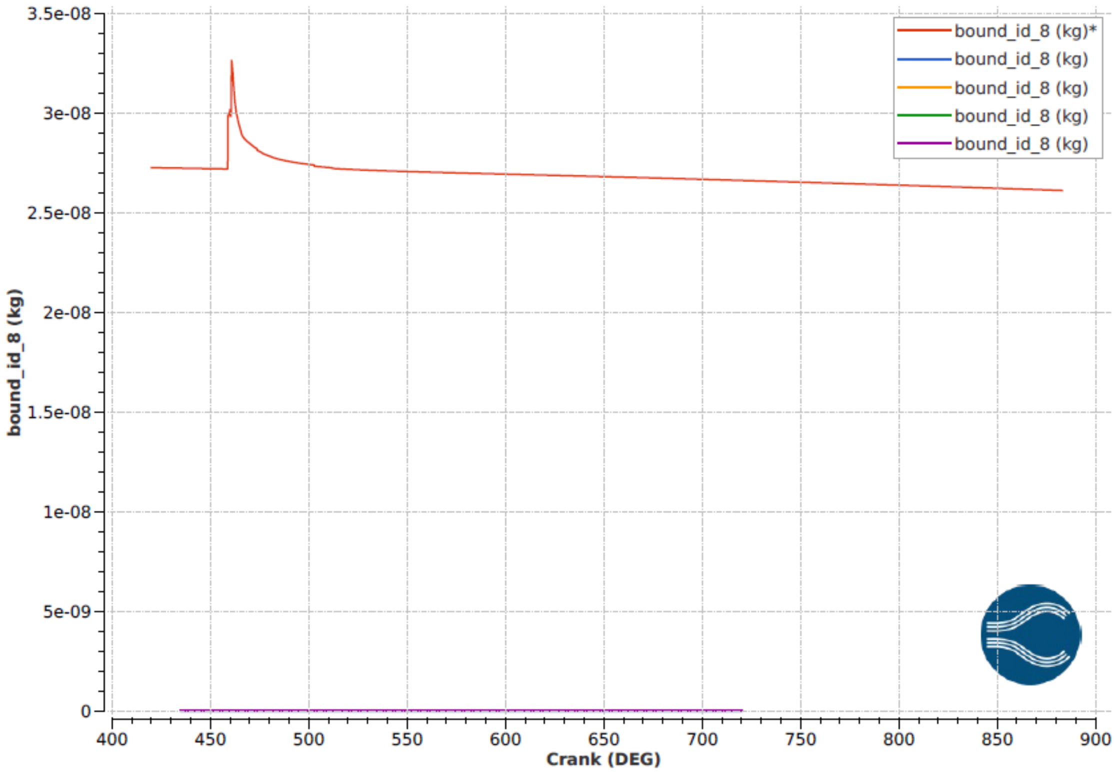

Figure 7 Time evolution of the amount of fuel spraying on the intake port (bound_id_8:Intake Port, red line: case 1, equilateral hexagon nozzle shape; blue line: case 2 equilateral triangle nozzle shape; orange line: case 2' equilateral triangle nozzle shape with deviated injector; green line: case 3, half droplet size; purple line: case 4, 5 times of scaling)

Same for exhaustive valve face (bound_id_18 in Converge CFD), compare to the cases conducted after case 1, the first case obviously shows much higher value than the rest, which means the change made also works on exhaustive valve face.

After adjusting the injector position back to the center of the entrance port, as shown in figure 7, 8 & 9, the third line has no significant change compared to the second line.

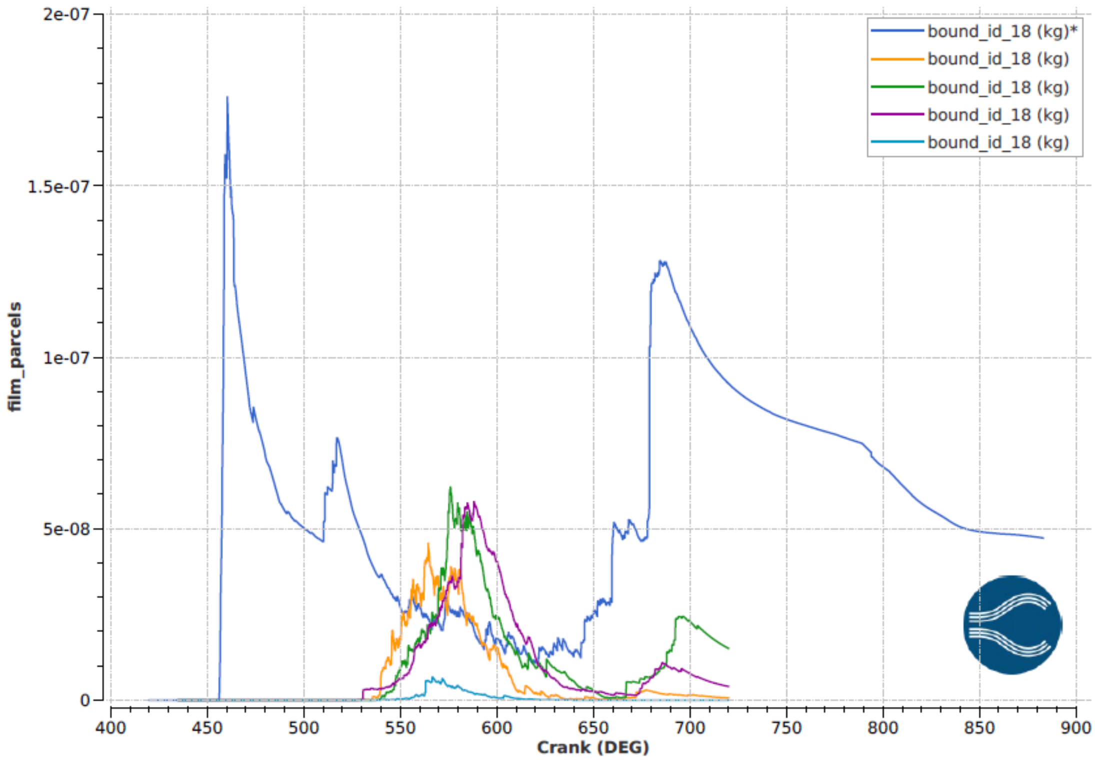

Figure 8 Time evolution of the amount of fuel spraying on the exhaustive valve face (bound_id_18: Exhaustive Valve Face, blue line: case 1, equilateral hexagon nozzle shape; orange line: case 2 equilateral triangle nozzle shape; green line: case 2' equilateral triangle nozzle shape with deviated injector; purple line: case 3, half droplet size; cyan line: case 4, 5 times of scaling)

4.2 Result by changing model size constant (droplet size)

Even though the situation mentioned in 4.1 is getting optimistic, comparing case 2 to case 1, the fuel spraying on liner obviously increases from 2e-06 to 3.25e-06, which means although the change made preciously improve the result for bound_id_8 (intake port), it meanwhile makes the situation for bound_id_5 worse (liner).

Since no obvious change happens after adjusting the nozzle shape and injector related parameters, droplet size turns to be another factor considered that may influence the fuel-air mixture. Intuitively, decreasing the size of droplet would make it easier for fuel to mix with air. Based on the default reference value, the droplet sizes in both RH model and RT model reduce to be half of the default value. This change does not have any impact on Intake Port, but it does make influence on liner and exhaust valve face as shown in figure 8 & 9. However, the change shown in the figure is not that obvious, which might mean droplet size is a factor that influence the fuel-air mixture formation but not the main one.

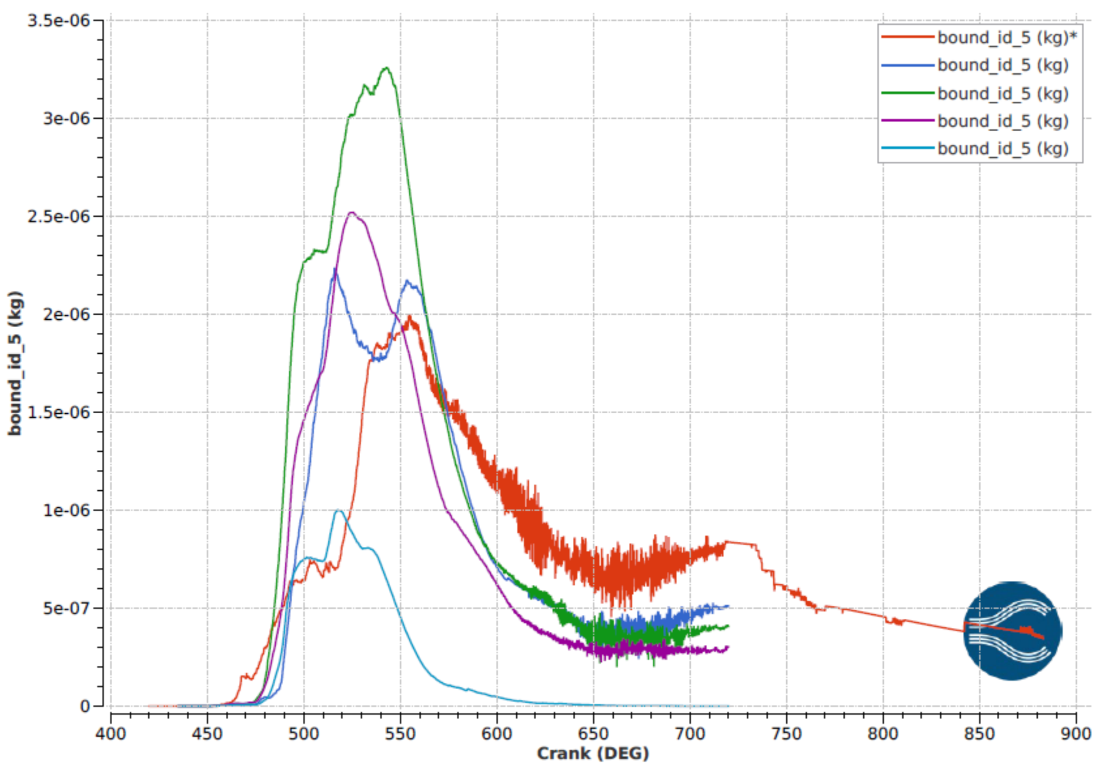

Figure 9 Time evolution of the amount of fuel spraying on the liner (bound_id_5: Liner, red line: case 1, equilateral hexagon nozzle shape; blue line: case 2 equilateral triangle nozzle shape; green line: case 2' equilateral triangle nozzle shape with deviated injector; purple line: case 3, half droplet size; cyan line: case 4, 5 times of scaling)

4.3 Result by changing scaling parameters

Another factor considered in this research is scaling including droplet heat transfer coefficient, droplet mass transfer coefficient, film heat transfer coefficient and film mass transfer coefficient, which control the transfer velocity of the variable mentioned above. By increasing these parameters, the process of turning droplet into vapor speeds up.

In figure 8 & 9, what can be seen is that the last line stays at the lowest position in the plot, which means least fuel sprays on facilities when increasing the scaling parameters.

4.4 Overall Equivalence Ratio

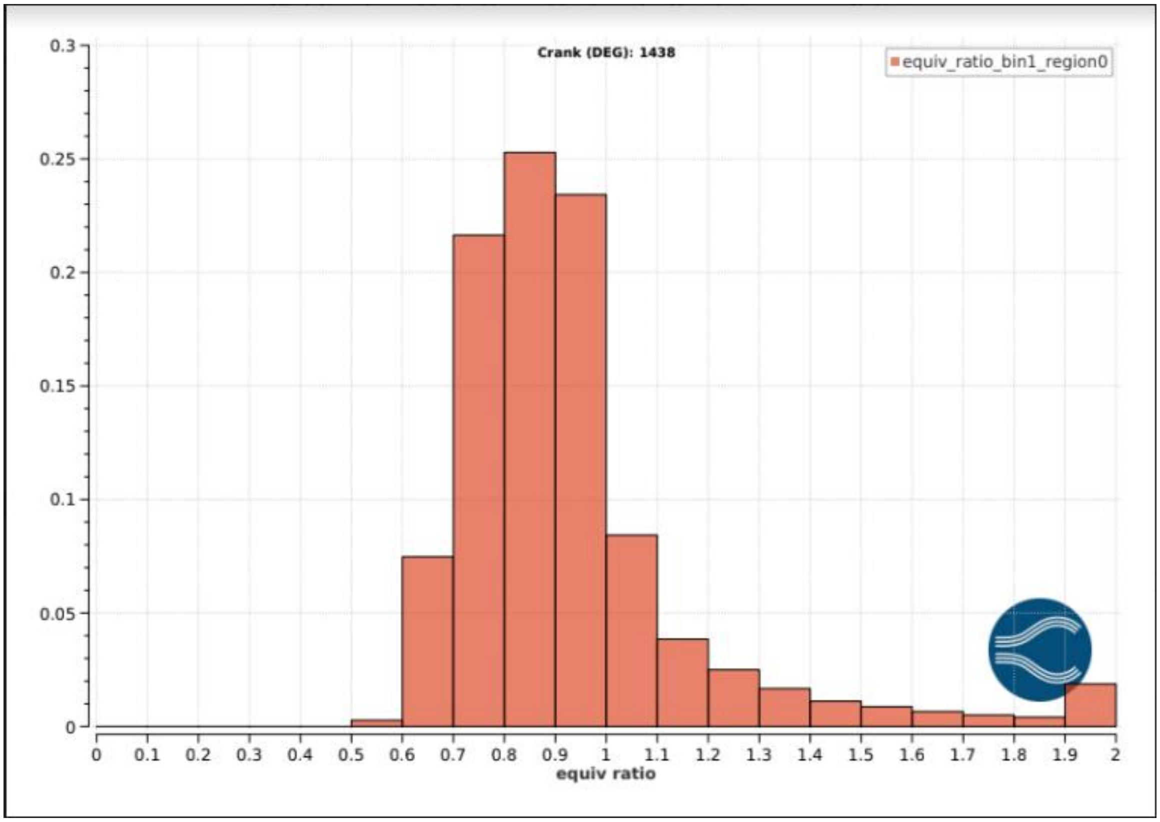

Figure 10 Distribution of the equivalence ratio for Case 1: Equilateral hexagon nozzle shape (region0: cylinder)

Figure 10 shows the equivalence ratio in case 1, the crank angle selected in this case is 1438, which is equivalent to 718 degrees as the spark angle. As shown in the figure, the possibility of equivalence ratio between 0.9 to 1 is just 0.23.

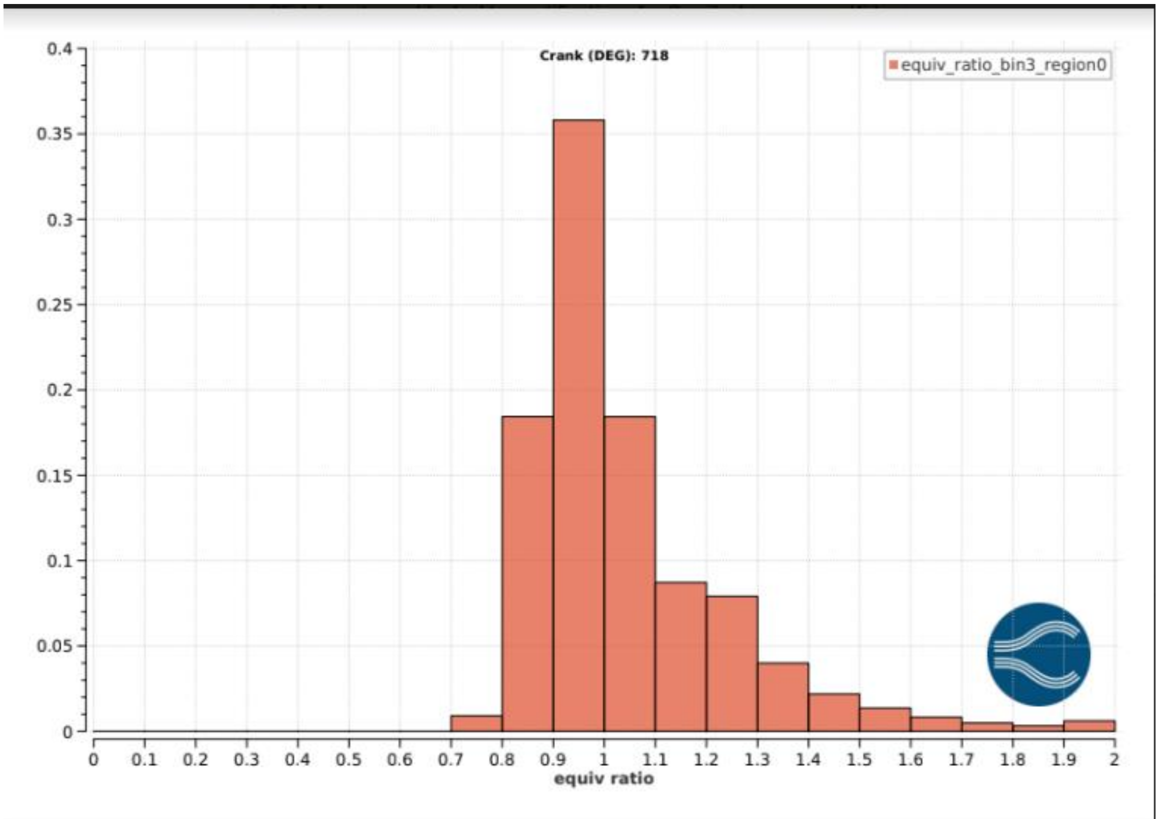

Figure 11 Distribution of the equivalence ratio for Case 2: Equilateral triangle nozzle shape (region0: cylinder)

Figure 11 shows the distribution of equivalence ratio in case 2. The possibility between 0.9 to 1 increases to 0.35. The equivalence ratio between 0.8 to 1.1 is 0.71, which is much better than case 1.

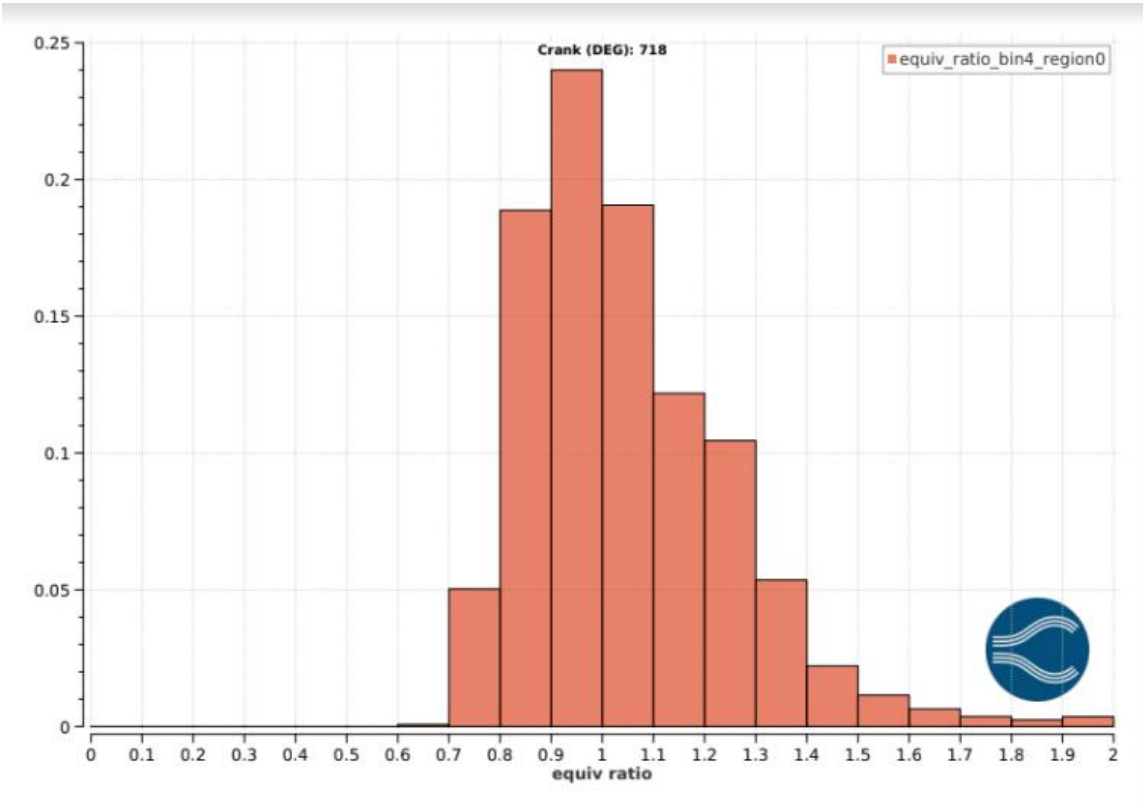

Figure 12 Distribution of the equivalence ratio for Case 3: Reduced model size constant (region0: cylinder)

Figure 12 shows the distribution of equivalence ratio in case 3. The possibility between 0.9 to 1 is 0.24. The equivalence ratio between 0.8 to 1.1 is 0.62.

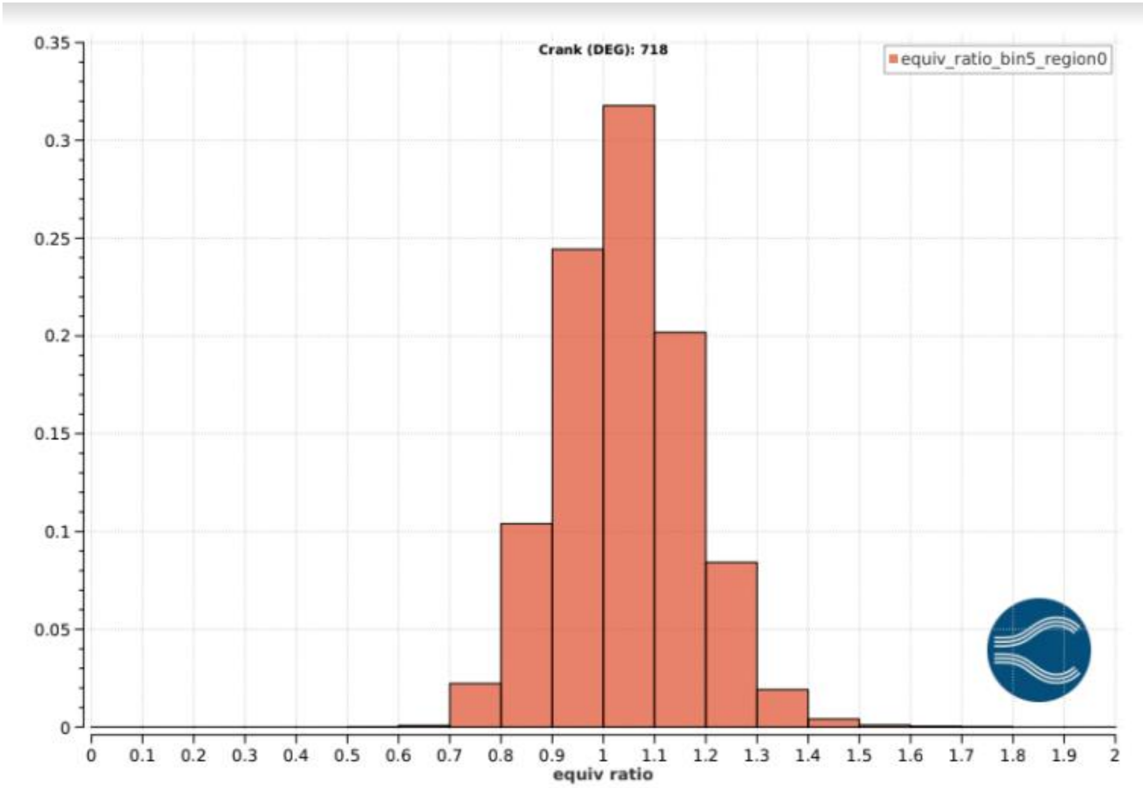

Figure 13 Distribution of the equivalence ratio for Case 4: Increased scaling (region0: cylinder)

Figure 13 shows the distribution of equivalence ratio in case 4. The possibility between 0.9 to 1 is 0.24. The equivalence ratio between 0.8 to 1.1 is 0.65.

In summary, in terms of equivalence ratio, case 2 shows the best performance result. According to the definition of equivalence ratio, when φ<1, it means less fuel exits in the cylinder than air. To approach a perfect case, other parameters still need adjusting to make φ as close to 1 as possible.

5. Conclusions

5.1 Summary

In this thesis, a cylinder with spray modeling is built based on the pre-built model available in Converge CFD. The parameters of the model are identified by using estimation either based on numerical simulation done by previous research, default reference value or experience. At this point, the simulation model performs much better than the pre-built model after adding spray modeling and adjusting related parameters. The model is correlated to a model experiment of an IC engine, which is used to calibrate the performance of the simulation model.

5.2 Major Conclusions

For the simulation model considered, changing the nozzle shape would largely influence the overall fuel spraying on the facilities but this also causes unexpected results including increasing the amount of fuel spraying on the liner. Droplet size is a factor that has impact on fuel-air mixture formation. However, according to the simulation result, the influence of this parameter on the final performance is not that evident. By increasing a droplet heat transfer coefficient, a droplet mass transfer coefficient, a film heat transfer coefficient and a film mass transfer coefficient, the rate for droplet changing from the liquid state to the vapor state largely increases, which improves the performance in an obvious extent.

5.3 Future Work

Ideally, the fuel should not be sprayed on the cylinder walls and other engine components, but is fully combusted. Currently, after adjusting the parameters mentioned in the thesis, the fuel spraying wasted decreases significantly, but the waste still exists, which means more work is needed to improve the situation.

In addition, the equivalence ratios of the simulations done so far are all much less than 1, which means that fuel and air are not perfectly mixed in the cylinder. Droplet size and the transfer efficient still need improving to identify a more ideal condition.

References

[1] U.S. Energy Information Administration. "FREQUENTLY ASKED QUESTIONS. How much gasoline does the United States consume?" (2017)

[2] Converge CFD SOFTWARE. "Converge Manual" (2017)

[3] M Takagi and Y Moriyoshi. "Modelling of A Hollow-Cone Spray at Different Ambient Pressures", Department of Electronics and Mechanical Engineering, Chiba University, Chiba, Japan. Int, J. Engine Res. Vol.5 No.1. (2003)

[4] P Adomeit and O Lang. S Pischinger. "Spray propagation and mixture formation in an air guided direct injection gasoline engine" (2000)